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Sent: Thursday, January 20, 2005 8:35 AM
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Subject: 1,2,3-Triochloropropane Properties
Attachments: Chemical Properties.pdf

Hi Steve,

Here's some information on the properties of 1,2,3-TCP to assist SAIC in updating their 1,2,3-TCP fact sheet. The information below is based on 1) a conversation I had with a soil gas sampling company (Environmental Support Technologies, Inc.; Curt knows of their reputation) representative, 2) data from internet web sites, and 3) internal CH2M HILL discussions and experience with 1,2,3-TCP.

1. 1,2,3-TCP should behave more like a VOC than an SVOC (semi-volatile organic compound). Attached are selected pages from the ChemFinder website (http://chemfinder.cambridgesoft.com/). These pages contain chemical property information for several chemicals that "behave" like VOCs. PCE, TCE, and 1,2,3-TCP are clearly VOCs, in particular because the methods used by labs to analyze groundwater samples for VOCs (e.g., 8260 and 524.2) have these as routine target compounds. 1,4-Dioxane is a borderline VOC/SVOC, in that it can be detected by the VOC laboratory analytical methods, but is more readily detected by SVOC laboratory analytical methods. As the term SVOC implies, 1,4-dioxane is not that volatile. And, this is one of the reasons why it is not readily amenable to soil gas surveys. However, what really affects the behavior of 1,4-dioxane and 1,2,3-TCP in the environment in the presence of water. From the attached data you'll see that 1,2,3-TCP is "insoluble" in water, with a solubility of 0.18 gm/100 mL. For comparison, TCE is less soluble in water at 0.11 gm/100 mL and PCE is even less soluble in water at 0.015 gm/100 mL. 1,4-dioxane on the other hand is "miscible" in water, which means that it "likes" to bond to water molecules, compared to sticking to itself in drops or pools in groundwater. What this all means is that 1,4-dioxane "likes" to be in groundwater and will not tend to volatilize into a vapor in the vadose zone (partially saturated region above the groundwater table) where it can be detected during soil gas sampling. At the other end of the spectrum, TCE and PCE, "aren't as happy" in groundwater and will tend to volatilize into vapor in the vadose zone, where they'll be detected during soil gas sampling. 1,2,3-TCP on the other hand falls somewhere in between the behavior of 1,4-dioxane and PCE/TCE. In other words (see below), it has a solubility that will allow it to volatilize into a vapor in the vadose zone, but not as readily as PCE or TCE. Another good web site with lots of chemical data is: http://webbook.nist.gov/chemistry/.
2. 1,2,3-TCP is amenable to detection via soil gas sampling. EST's representative said that they have analyzed for this compound during soil gas surveys, although they certainly don't target this compound for detection and analysis as often as say PCE and TCE. His recollection was that they had not detected 1,2,3-TCP during any of their surveys. There is no way of knowing why they haven't detected 1,2,3-TCP: whether it's not present, too low in concentration to be detected, or not easily detected. However, EST has detected the petroleum hydrocarbon naphthalene during soil gas surveys. This makes sense, since napthalene is less soluble in water than 1,2,3-TCP (see attached PDF file). However, another property that can influence the ability to detect a compound during soil gas surveys is the boiling point of a chemical or liquid. Water, which has a boiling point of 100 degrees centigrade, easily evaporates into a vapor. 1,2,3-TCP, with a boiling point of 156 degrees centigrade, evaporates with a bit more difficulty into a vapor, and napthalene, with a boiling point of 218 degrees centigrade requires even more heating to evaporate. So, the fact that napthalene vapors can be detected during soil gas sampling suggests that 1,2,3-TCP vapors should be detectable during soil gas sampling. For comparison, PCE and TCE, which are readily detected during soil gas sampling, have lower boiling points (closer to or less than water; see attached PDF), and vaporize relatively easily compared to 1,2,3-TCP and napthalene.
3. 1,2,3-TCP has been detected at sites around the U.S. As I mentioned previously, it's been detected in the Burbank OU in the San Fernando Valley here in southern California. The attached link shows that 1,2,3-TCP has been detected, in particular in soil gas, at a site in New York. Understanding the behavior and detections of 1,2,3-TCP at other sites will help us to understand its fate and transport in Area 3.

4. As a contaminant migrating in groundwater, 1,2,3-TCP will behave in a manner similar to other VOCs like PCE and TCE. From the realm of groundwater treatment, 1,2,3-TCP is not readily removed by air stripping treatment. PCE and TCE are much easier to remove from groundwater via air stripping. These behaviors are consistent with 1,2,3-TCP's "desire" to dissolve more easily into water and it's tendency to be more difficult to vaporize during boiling. On the other hand, 1,2,3-TCP is readily removed from groundwater that is passed through beds of granular activated carbon for treatment. In this case, 1,2,3-TCP behaves like PCE and TCE, in that all three chemicals will have tendency to stick to carbon that might be present in a groundwater aquifer, such as in the form of organic plant matter from trees, plants, leaves, moss, etc. deposited along with sediments in lakes, rivers, and streams. What this all means is that 1,2,3-TCP migration in a groundwater aquifer will be "slowed down" or "retarded" compared to the movement of a water molecule or a chemical like chloride ion, which does not readily react with, sorb to, and be retarded by organic carbon in an aquifer.

Please let me know if you have questions about the information in this e-mail.

Thanks,

Bob

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